

Distribution functions, extremal limits and optimal transport

Dedicated to the 125th anniversary of J.G. van der Corput

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Abstract

Encouraged by the study of extremal limits for sums of the form

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N c(x_n, y_n)$$

with uniformly distributed sequences $\{x_n\}$, $\{y_n\}$ the following extremal problem is of interest

$$\max_{\gamma} \int_{[0,1]^2} c(x, y) \gamma(dx, dy),$$

for probability measures γ on the unit square with uniform marginals, i.e., measures whose distribution function is a copula.

The aim of this article is to relate this problem to combinatorial optimization and to the theory of optimal transport. Using different characterizations of maximizing γ 's one can give alternative proofs of some results from the field of uniform distribution theory and beyond that treat additional questions. Finally, some applications to mathematical finance are addressed.

1 Introduction and motivation

In a series of papers J.G. van der Corput [47, 48] systematically investigated distribution functions of sequences of real numbers. Some of his main results are as follows:

- (i) Any sequence of real numbers has a distribution function.
- (ii) Any everywhere dense sequence of real numbers can be rearranged in such a way that the new sequence has an arbitrarily given distribution function.

Clearly, in general a distribution function is not uniquely determined by the sequence. Furthermore, van der Corput established necessary and sufficient conditions for a set \mathcal{M} of non-decreasing functions such that \mathcal{M} is the set of distribution functions of some sequence of real numbers.

More recently, the study of distribution functions was extended to multivariate functions by the Slovak school of O. Strauch and his coworkers; see [5, 6, 24, 44]. In particular, they studied properties of the set of distribution functions of sequences in $[0, 1]^2$ and various extremal problems related to distribution functions. It should be noted that bi-variate distribution functions are well-known in financial mathematics for modeling dependencies in risk processes.

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From Fialová & Strauch [23, Thm 1] one knows that for uniformly distributed sequences $\{x_n\}$, $\{y_n\}$ in $[0, 1]$ and a continuous function $c : [0, 1]^2 \rightarrow \mathbb{R}$ one has

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N c(x_n, y_n) = \int_{[0,1]^2} c(x, y) \gamma(dx, dy), \quad (1)$$

where γ is a probability measure on the unit square equipped with the σ -algebra of Borel sets. Such a measure exhibits a bi-variate distribution function $C : [0, 1]^2 \rightarrow [0, 1]$ which is generally called a *copula*. The aim of this article is to provide a connection between the problem of finding extremal limits in (1) (or maximal and minimal bounds for such limits) by studying the optimization problem

$$\int_{[0,1]^2} c(x, y) \gamma(dx, dy) \mapsto \max \quad (2)$$

and the field of optimal transport. Indeed, we will show how this problem can be perfectly embedded in the general theory of optimal transport.

Motivated by the discussion on the limiting property (1) problem (2) attracted some attention in the number theoretic community and found its way on the collection of unsolved problems of *Uniform Distribution Theory*¹. We will mention some existing results in that context below. Notice that in the uniform distribution literature, problem (2) is originally written as an optimization with respect to functions $C : [0, 1]^2 \rightarrow [0, 1]$ satisfying the following properties: for every $x, y \in [0, 1]$

$$\begin{aligned} C(x, 0) &= C(0, y) = 0, \\ C(x, 1) &= x \text{ and } C(1, y) = y, \end{aligned}$$

and for every $x_1, x_2, y_1, y_2 \in [0, 1]$ with $x_2 \geq x_1$ and $y_2 \geq y_1$

$$C(x_2, y_2) - C(x_2, y_1) - C(x_1, y_2) + C(x_1, y_1) \geq 0.$$

Clearly, in this particular situation a copula is a bivariate distribution function on $[0, 1]^2$ with standard uniform marginals. From the above stated properties one additionally sees that a copula C induces a (Borel-)probability measure γ on $[0, 1]^2$, via the formula

$$\gamma([a, b] \times [c, d]) = C(b, d) - C(b, c) - C(a, d) + C(a, c).$$

A first result in the direction of extremal limits (1) is given in [35], where the authors take $c(x, y) = |x - y|$ in order to find optimal upper and lower bounds on the average distance between consecutive points of u.d. sequences. In particular, they proved $\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} |x_{n+1} - x_n| = \frac{2(b-1)}{b^2}$ for the van der Corput sequence $(\phi_b(n))_{n \geq 0}$ in base b .

By looking at the same problem, but in the formulation of (2), the authors in [23] could give an explicit formula for the asymptotic distribution function of the sequence $(\phi_b(n), \phi_b(n+1))_{n \geq 0}$, that is of the copula $C(x, y)$.

The problem of finding the limit distribution of consecutive elements of the van der Corput sequence was also considered in [1], but using a different approach based on ergodic properties of the sequence itself. However, this approach does not give an explicit form of the copula $C(x, y)$. This last problem is not easy to handle with and, apart from the already mentioned papers [23, 35], only [22] is known, where the authors found an explicit asymptotic distribution function of the sequence $(\phi_b(n), \phi_b(n+1), \phi_b(n+2))_{n \geq 0}$.

Problem (2) has been recently studied in [25] in connection with a well-known problem in combinatorial optimization, namely the linear assignment problem. By means of this tool, the authors

¹Problem 1.29 in the open problem collection as of 28. November 2013 (<http://www.boku.ac.at/MATH/udt/unsolvedproblems.pdf>)

give optimal upper and lower bounds for integrals of two-dimensional, piecewise constant functions with respect to copulas and construct the copulas for which these bounds are attained. More precisely, the copulas realizing these bounds are shuffles of M , where the permutation σ is the one which solves the assignment problem.

From the uniform distribution point of view, this class of copulas represents a family of uniform distribution preserving mappings (u.d.p.), i.e. maps f generating u.d. sequences $(f(x_n))_{n \in \mathbb{N}}$ for every u.d. sequence $(x_n)_{n \in \mathbb{N}}$. We will discuss more extensively the linear assignment problem and the algorithm that solves it in one of the following next sections.

The problem (2) is known as Monge-Kantorovich transport problem. Its origin is the question of how to transport soil from one location to another at minimal costs. More precisely, suppose these two locations are disjoint subsets M and F of the Euclidean plane \mathbb{R}^2 and that $c(x, y): \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow [0, \infty)$ is the cost of transporting one shipment of soil from x to y . For simplicity, we assume that there is no splitting of shipments. Thus, a transport map is a function $T: M \rightarrow F$. The goal is to find the optimal transport map which minimizes the total costs

$$c(T) := \sum_{m \in M} c(m, T(m)),$$

under the restriction that all the soil needs to be moved. We will give a precise description of the optimal transport problem and fundamental results in section 3.

The Monge-Kantorovich problem has found a great variety of applications in pure and applied mathematics, such as Ricci curvature [29], nonlinear partial differential equations [12], gradient flows [3], structure of cities [15], maximization of profits [14], leaf growth [50] and so on.

As a prominent field of application of the theory of copulas and the transport problem one needs to mention financial mathematics. In the last decade copulas, or more precisely some parametrized families of copulas, became very popular in finance for modelling dependence structures within groups of assets or more generally between different kinds of risk factors. In the past the study of dependence structures was typically reduced to the determination of correlation coefficients. However, correlation coefficients describe dependencies perfectly only in the situation of marginally normal distributed risk factors, while distributions obtained from financial market data are typically not normal. A standard introduction to risk modeling and particularly to practical aspects of copula modeling is the book by McNeil et al. [30].

It turned out that a precise description of the dependency structure within a portfolio of risks is not feasible in practice. That's why one is trying to determine some (one may call it worst case or robust) bounds on risk measures of portfolios. For this purpose it is possible to utilize variants of the optimal transport problem: *try to minimize a risk measure of a portfolio of several risks with respect to their distribution while preserving their marginals*. Some recent publications studying problems from risk management are Rüschendorf [40], Puccetti & Rüschendorf [36] or Bernard et al. [11]. A paper dealing with model independent bounds on option prices using theory of optimal transport is Beiglböck et al. [7].

2 Mathematical formulation

In this section we give precise statements of the mathematical objects at hand. We refer to [18, 21, 26, 33] for details. Our starting point is Sklar's Theorem (see e.g. [33, Theorem 3.2.2]), a classical result about copulas which provides the theoretical foundation for application of copulas.

Theorem 2.1

Given a d -dimensional distribution function (d.f.) H with marginals F_1, \dots, F_d , there exists a

d -copula C such that for all $(x_1, x_2, \dots, x_d) \in \mathbb{R}^d$

$$H(x_1, x_2, \dots, x_d) = C(F_1(x_1), F_2(x_2), \dots, F_d(x_d)) \quad (3)$$

The copula C is uniquely defined on $\prod_{j=1}^d \text{Ran}(F_j)$ and is therefore unique if all the marginals are continuous (here $\text{Ran}(F_j)$ denotes the range of F_j).

Conversely, if F_1, F_2, \dots, F_d are d (1-dimensional) d.f.'s, then the function H defined through Eq. (3) is a d -dimensional d.f..

Given a d -variate d.f. F , one can derive a copula C . Specifically, when the marginals F_i are continuous, C can be obtained by means of the formula

$$C(u_1, u_2, \dots, u_d) = F(F_1^{-1}(u_1), F_2^{-1}(u_2), \dots, F_d^{-1}(u_d)) ,$$

where $F_i^{-1} = \inf\{t | F_i(t) \geq s\}$ is the pseudo-inverse of F_i .

Thus, copulas are essentially a way for transforming the r.v. (X_1, X_2, \dots, X_d) into another r.v. $(U_1, U_2, \dots, U_d) = (F_1(X_1), F_2(X_2), \dots, F_d(X_d))$ having uniform margins on $[0, 1]$ and preserving the dependence among the components. As we have seen in Section 1, every copula C induces a probability measure γ . Moreover, there is a one-to-one correspondence between copulas and doubly stochastic measures. For every copula C , the measure γ is doubly stochastic in the sense that for every Borel set $B \subset [0, 1]$, $\gamma([0, 1] \times B) = \gamma(B \times [0, 1]) = \lambda(B)$ where λ is the Lebesgue measure on $[0, 1]$. Conversely, for every doubly stochastic measure μ , there exists a copula C given by $C(u, v) = \mu([0, u] \times [0, v])$. Clearly, a probability measure on $([0, 1]^2, \mathcal{B}([0, 1]^2))$ with uniform marginals is doubly stochastic. Therefore, we can translate some measure-theoretic concepts and results into the language of copulas.

In particular, we are interested in the correspondence between copulas C and measure-preserving transformations f, g on the unit interval, via the formula

$$C_{f,g}(u, v) = \lambda(f^{-1}[0, u] \cap g^{-1}[0, v]) .$$

We refer to [17] for details and the study of related properties.

The following theorem shows how every copula can be bounded from above and below. The upper and lower bounds are called Fréchet-Hoeffding bounds.

Theorem 2.2

Suppose F_1, \dots, F_d are marginal d.f.'s and F is any joint d.f. with those given marginals, then for all $\mathbf{x} \in \mathbb{R}^d$,

$$\left(\sum_{k=1}^d F_k(x_k) + 1 - d \right)^+ \leq F(\mathbf{x}) \leq \min(F_1(x_1), \dots, F_d(x_d)) . \quad (4)$$

The right-hand side of (4) is always a copula, whereas the left-hand side is a copula only $d = 2$, see [26, Theorem 3.2 and 3.3].

Thus, the problem is to find bounds of the form

$$\int_{[0,1]^2} c(x, y) dC_{\min}(x, y) \leq \int_{[0,1]^2} c(x, y) dC(x, y) \leq \int_{[0,1]^2} c(x, y) dC_{\max}(x, y), \quad (5)$$

where C_{\min}, C_{\max} are copulas.

A particularly interesting subclass of copulas for our problems are so-called shuffles of M , see [33, Section 3.2.3]. They represent a construction principle that generates new copulas by means of a suitable rearrangement of the mass distribution of the upper Fréchet bound M .

Definition 2.3 (Shuffles of M)

Let $n \geq 1$, $s = (s_0, \dots, s_n)$ be a partition of the unit interval with $0 = s_0 < s_1 < \dots < s_n = 1$, π be a permutation of $S_n = \{1, \dots, n\}$ and $\omega: S_n \rightarrow \{-1, 1\}$. We define the partition $t = (t_0, \dots, t_n)$, $0 = t_0 < t_1 < \dots < t_n = 1$ such that each $[s_{i-1}, s_i] \times [t_{\pi(i)-1}, t_{\pi(i)}]$ is a square. A copula C is called shuffle of M with parameters $\{n, s, \pi, \omega\}$ if it is defined in the following way: for all $i \in \{1, \dots, n\}$ if $\omega(i) = 1$, then C distributes a mass of $s_i - s_{i-1}$ uniformly spread along the diagonal of $[s_{i-1}, s_i] \times [t_{\pi(i)-1}, t_{\pi(i)}]$ and if $\omega(i) = -1$ then C distributes a mass of $s_i - s_{i-1}$ uniformly spread along the antidiagonal of $[s_{i-1}, s_i] \times [t_{\pi(i)-1}, t_{\pi(i)}]$.

Note that the two Fréchet-Hoeffding bounds W, M are trivial shuffles of M with parameters $\{1, (0, 1), (1), -1\}$ and $\{1, (0, 1), (1), 1\}$, respectively. Furthermore it is well-known that every copula can be approximated arbitrarily close with respect to the supremum norm by a shuffle of M ; see e.g. [33, Theorem 3.2.2].

In [20, Theorem 4] shuffles of M are characterized in terms of measure preserving transformations T of $[0, 1]$ and the push-forward of the doubly stochastic measure induced by M . More precisely, the authors proved the following result.

Theorem 2.4

Let γ_C denote the doubly stochastic measure induced by the copula C and γ_M be the doubly stochastic measure induced by M . The following statements are equivalent:

- (a) a copula C is a shuffle of M ;
- (b) there exists a piecewise continuous measure-preserving permutation such that $\gamma_C = S_T * \gamma_M$, where $S_T : [0, 1]^2 \rightarrow [0, 1]^2$ is defined as $S_T(u, v) = (T(u), v)$ for every $(u, v) \in [0, 1]^2$.

On the other hand, the general problem is that of determining curves in the unit square which can be considered as the support of a copula. In [31] it has been proven that, for every copula obtained as a shuffle of M , there is a piecewise linear function whose graph supports the probability mass. In this context, the following general result holds.

Proposition 2.5

Let $f : [0, 1] \rightarrow [0, 1]$ be a Borel measurable function. Then, there exists a copula C whose associated measure γ has its mass concentrated on the graph of f (with $\gamma(G(f)) = 1$) if, and only if, the function f preserves the Lebesgue measure λ .

These results provide an interesting link between the theory of copulas and the theory of uniform distribution of sequences of points. In particular, shuffles of M can be considered as special uniform distribution preserving (u.d.p.) mappings. Recently, different concepts of convergence for copulas have been used; the question arising in this context is about the closure of the class of shuffles of M with respect to different notions of convergence and thus topologies. This problem has been considered for instance in [19].

Now we consider the connection between copulas and uniformly distributed sequences of points in $[0, 1]$. For a detailed account on this concept the interested reader is referred to Drmota & Tichy [18].

Definition 2.6

A sequence $(x_n)_{n \in \mathbb{N}}$ of points in $[0, 1]$ is called uniformly distributed (u.d.) if and only if

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \mathbf{1}_{[a, b]}(x_n) = b - a$$

for all intervals $[a, b] \subseteq [0, 1]$, where $\mathbf{1}_E$ denotes as usual the indicator function of the set E .

We call C the asymptotic distribution function (a.d.f.) of a point sequence $(x_n, y_n)_{n \in \mathbb{N}}$ in $[0, 1]^2$ if

$$C(x, y) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N \mathbf{1}_{[0, x] \times [0, y]}(x_n, y_n),$$

holds in every point (x, y) of continuity of C . In [23] Fialová and Strauch consider

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N f(x_n, y_n),$$

where $(x_n)_{n \geq 1}, (y_n)_{n \geq 1}$ are u.d. sequences in the unit interval and f is a continuous function on $[0, 1]^2$. In this case the a.d.f. g of $(x_n, y_n)_{n \geq 1}$ is always a copula and we can write

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N f(x_n, y_n) = \int_0^1 \int_0^1 f(x, y) dg(x, y). \quad (6)$$

The following theorem proved in Tichy & Winkler [45] is of particular relevance for us in order to show the connection between uniform distribution preserving maps and approximations by means of shuffles of M [31].

Theorem 2.7

The set of all continuous piecewise linear u.d.p. mappings are dense in the set of all continuous u.d.p. mappings with respect to uniform convergence.

3 Theory of optimal transport

In this section we briefly state fundamental results from the theory of the Monge-Kantorovich optimal transport problem. The presented results on existence of optimizers and the dual problem formulation are stated in an adequate depth such that the number theoretic questions under consideration are covered. Comprehensive accounts on the subject are Villani [49] or Rachev & Rüschendorf [37] for example, a set of lecture notes on the topic would be Ambrosio & Gigli [2]. For the basic presentation of the optimal transport problem we are following the above mentioned references.

3.1 Problem formulation

Let X and Y be Polish spaces and denote $\mathcal{P}(X)$ the set of all Borel probability measures on X ($\mathcal{P}(Y)$ on Y). For a Borel-measurable map $T : X \rightarrow Y$ and $\mu \in \mathcal{P}(X)$, the measure $T_{\#}\mu \in \mathcal{P}(Y)$ defined by

$$T_{\#}\mu(E) = \mu(T^{-1}(E)) \quad \text{for } E \in \mathcal{B}(Y)$$

is called the *push forward of μ through T* . Together with a Borel measurable cost function $c : X \times Y \rightarrow \mathbb{R} \cup \{+\infty\}$ we can give:

Monge formulation: Let $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ and minimize

$$\int_X c(x, T(x)) \mu(dx) \quad (7)$$

among all *transport maps* T from μ to ν (all maps for which $T_{\#}\mu = \nu$). The transport map T has the meaning that a unit mass is put from the point x to the point $y = T(x)$ and at the same time

the distribution ν is achieved.

The relaxation of Monge's optimal transport problem is the following:

Kantorovich formulation: Let $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ and minimize

$$\int_{X \times Y} c(x, y) \gamma(dx, dy) \quad (8)$$

in the set of $ADM(\mu, \nu)$ of all *transport plans* $\gamma \in \mathcal{P}(X \times Y)$ from μ to ν , i.e., the set of all Borel probability measures on $X \times Y$, such that

$$\begin{aligned} \gamma(A \times Y) &= \mu(A) \quad \forall A \in \mathcal{B}(X), \\ \gamma(X \times B) &= \nu(B) \quad \forall B \in \mathcal{B}(Y). \end{aligned}$$

Now the meaning of a transport plan is that $\gamma(A \times B)$, for $A \in \mathcal{B}(X)$ and $B \in \mathcal{B}(Y)$, denotes the mass initially placed in A which is moved into B , in contrast to transport maps a unit mass can now be split. One can immediately answer the question of existence of an optimizer.

Theorem 3.1 (Th. 1.5 from [2])

Assume c is lower semicontinuous, then there exists a minimizer for problem (8).

The following theorem is an excerpt from Theorem 5.10 of Villani [49], it will give us the right tools for the construction of optimal solutions for some particular examples. But at first we need some notions from [37, 49].

Definition 3.2 (c -cyclical monotonicity)

A set $\Gamma \subset X \times Y$ is c -cyclically monotone if for all $(x_n, y_n) \in \Gamma$ with $1 \leq n \leq N$ for $N \in \mathbb{N}$, $x_{N+1} = x_1$, it holds that

$$\sum_{n=1}^N c(x_n, y_n) \leq \sum_{n=1}^N c(x_{n+1}, y_n).$$

Definition 3.3 (c -convexity)

Let X, Y be sets and $c : X \times Y \rightarrow \mathbb{R} \cup \{+\infty\}$, a function $f : X \rightarrow \mathbb{R} \cup \{+\infty\}$ is c -convex if it is not identically $+\infty$ and there exists $a : Y \rightarrow \mathbb{R} \cup \{\pm\infty\}$ such that

$$f(x) = \sup_{y \in Y} [a(y) - c(x, y)] \quad \text{for all } x \in X.$$

Its c -transform is defined by

$$f^c(y) = \inf_{x \in X} [f(x) + c(x, y)] \quad \text{for all } y \in Y,$$

and its c -subdifferential is the set

$$\delta_c f = \{(x, y) \in X \times Y \mid f^c(y) - f(x) = c(x, y)\},$$

or at given $x \in X$

$$\delta_c f(x) = \{y \in Y \mid f^c(y) - f(x) = c(x, y)\}.$$

Now everything is clarified such that we can state the theorem.

Theorem 3.4 (Th. 5.10 ii) [49])

Let X and Y be Polish spaces, $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$. Let the cost function $c : X \times Y \rightarrow \mathbb{R} \cup \{+\infty\}$ be lower semicontinuous such that $c(x, y) \geq a(x) + b(y)$ for all $(x, y) \in X \times Y$ for some real-valued upper semicontinuous functions $a \in L^1(\mu)$ and $b \in L^1(\nu)$. Furthermore assume that (8) is finite, then there is a measurable c -cyclically monotone set $\Gamma \subset X \times Y$ such that for any $\gamma \in ADM(\mu, \nu)$ the following statements are equivalent:

- (a) γ is optimal,
- (b) γ is concentrated on a c -cyclically monotone set,
- (c) there is a c -convex function f such that, γ -a.s. $f^c(y) - f(x) = c(x, y)$,
- (d) γ is concentrated on Γ .

Another variant - or better formulation - of problem (8) is through a coupling of random variables. This formulation is of more probabilistic nature and perfectly suits applications from mathematical finance.

Coupling formulation: At first the ‘inf’ from (8) is turned into a ‘sup’, according to a standard presentation from Rüschendorf [39]. Secondly instead of *transport plan* the notion *coupling* is used, i.e. coupling of two random variables with fixed marginal distributions. Then one may write problem (8) as, cf.[39, Sec. 4.2],

$$\sup\{\mathbb{E}(c(X_1, X_2)) \mid X_1, X_2 \text{ couplings of } \mu, \nu \text{ with } P_{X_1} = \mu \text{ and } P_{X_2} = \nu\}. \quad (9)$$

The supremum is taken over the set of all bivariate $X \times Y$ -valued random variables (X_1, X_2) with given marginal distributions μ and ν . Consequently, $\gamma \in ADM(\mu, \nu)$ corresponds to the bivariate distribution of (X_1, X_2) .

For translating Theorem 3.4 to this maximization situation one needs to adapt the c -convexity notion. Now a function $f : X \rightarrow \mathbb{R}$ is called c -convex if it has a representation $f(x) = \sup_y \{c(x, y) + a(y)\}$, for some function a . The c -subdifferential of f at x is directly (hiding the c -transform) given by

$$\partial_c f(x) = \{y \mid f(z) - f(x) \leq c(z, y) - c(x, y) \ \forall z \in X\}$$

and $\partial_c f = \{(x, y) \in X \times Y \mid y \in \partial_c f(x)\}$.

Under the assumptions of Theorem 3.4 for X, Y and lower semicontinuity of c one gets an analogous statement.

Theorem 3.5 (Th. 4.7 from [39])

Let c be such that $c(x, y) \geq a(x) + b(y)$ for some $a \in L^1(\mu)$, $b \in L^1(\nu)$ and assume finiteness of (9). Then a pair (X_1, X_2) with $X_1 \stackrel{d}{\sim} \mu$, $X_2 \stackrel{d}{\sim} \nu$ is an optimal c -coupling between μ and ν if and only if

$$(X_1, X_2) \in \partial_c f \text{ a.s.}$$

for some c -convex function f , equivalently, $X_2 \in \delta_c f(X_1)$ a.s.

Uniform Marginals

In the following sections we will apply Theorem 3.4 to problems in the spirit of [23] and in particular to problem (2). Therefore in these applications we choose $X = Y = [0, 1]$, fix the marginal distributions to be uniform $\mu = \nu = \mathcal{U}[0, 1]$ and choose the cost function $c : [0, 1]^2 \rightarrow \mathbb{R}$ to be continuous. For this setting Theorem 3.4 applies and (8) is clearly finite. In this setting the Monge problem is an optimization problem with respect to uniform distribution preserving maps.

Remark 3.1

In general the question if an optimal transport plan in the Kantorovich formulation (8) is induced by an optimal transport map from the Monge formulation (7) is not answered in the corresponding literature. But there are some particular situations which allow for affirmative results. For instance for Borel measures μ, ν on \mathbb{R}^d , $c(x, y) = h(x - y)$ for a strictly convex function h and μ absolutely continuous with respect to Lebesgue measure there exists a unique map s such that the measure $\gamma = (\text{id} \times s)_\# \mu$ is optimal. For the situation of one dimensional marginals several examples of a similar structure are given in Uckelmann [46] and Rüschendorf & Uckelmann [41].

Theorem 3.4 or its complete formulation which is Theorem 5.10 from Villani [49] heavily rely on a dual problem formulation. How far the duality relation can be exploited, i.e., up to which parameter configuration the value of the primal solution equals the value of dual solution, is recently discussed in Beiglböck & Schachermayer [10] and Beiglböck et al. [8].

3.2 Application of Theorem 3.4

Now we are ready to give two applications of Theorem 3.4. The first one, dealing with a result from [23], concerns a direct verification of optimality via the c -cyclical monotonicity property. The second one treats an open problem from [43] by constructing explicitly a c -convex function.

We start by studying Theorem 5. from Fialová & Strauch [23] from the transport point of view.

Theorem 3.6 ([23])

Let $c : [0, 1]^2 \rightarrow \mathbb{R}$ be a Riemann integrable function with $\frac{\partial^2 c}{\partial x \partial y} > 0$ for all $(x, y) \in (0, 1)^2$. Then

$$\begin{aligned} \max_{\gamma - \text{copula}} \int_0^1 \int_0^1 c(x, y) \gamma(dx, dy) &= \int_0^1 c(x, x) dx, \\ \min_{\gamma - \text{copula}} \int_0^1 \int_0^1 c(x, y) \gamma(dx, dy) &= \int_0^1 c(x, 1 - x) dx, \end{aligned}$$

where the maximum is attained in $\gamma^u = \min\{x, y\}$ and the minimum in $\gamma^l(x, y) = \max\{x + y - 1, 0\}$, uniquely.

Remark 3.2

The maximum and the minimum are attained at the co-called upper and lower Fréchet bounds. Now by means of the c -cyclical monotonicity criterion for optimality we can give an alternative proof of the Theorem above. The procedure is similar to the one used in the proof of Proposition 1. from Rochet [38] in a slightly different context. Rochet proves that if the derivative condition is fulfilled the support of a transport plan $\Gamma(x)$ is c -cyclically monotone if and only if $\Gamma(\cdot)$ is non-decreasing. Combining this with a result on uniform distribution preserving maps from Tichy & Winkler [45] one arrives at Fialová & Strauch's result that $\Gamma(x) = x$ is the maximizing transport plan and $\Gamma(x) = 1 - x$ is the minimizing one.

Notice Theorem 3.1.2. from [37] includes the situations of Theorem 5. and 6. from Fialová & Strauch [23].

Proof: We need to show that for $N \in \mathbb{N}$ and x_0, x_1, \dots, x_N

$$\sum_{n=0}^N c(x_{n+1}, y_n) - c(x_n, y_n) \leq 0,$$

where $x_{N+1} = x_0$ and (x_n, y_n) are in the support of the to be shown optimal measure. In our particular situation for the upper bound $y_n = \Gamma(x_n) = x_n$. We start with a cycle of length 2

($N = 1$) and points x_0, x_1 and assume w.l.o.g $x_1 > x_0$. From

$$c(x_0, x_1) - c(x_1, x_1) + c(x_1, x_0) - c(x_0, x_0) = - \int_{x_0}^{x_1} \int_{x_0}^{x_1} \frac{\partial^2 c}{\partial x \partial y}(x, y) dy dx \leq 0$$

the statement follows. Now assume that for all cycles of length N the statement holds true,

$$\sum_{n=0}^{N-1} c(x_{n+1}, x_n) - c(x_n, x_n) \leq 0,$$

and choose arbitrary x_0, x_1, \dots, x_N (again w.l.o.g. $x_N = \max_{n \in \{0, 1, \dots, N\}} x_n$). Fix a sub-cycle of length $N - 1$ with $x'_n = x_n$ for $0 \leq n \leq N - 1$ and $x'_N = x_0$. Then using

$$A := \sum_{n=0}^{N-1} c(x'_{n+1}, x'_n) - c(x'_n, x'_n) \leq 0,$$

we get ($x_{N+1} = x'_N = x_0$),

$$\begin{aligned} \sum_{n=0}^N c(x_{n+1}, x_n) - c(x_n, x_n) &= A + [c(x_N, x_{N-1}) - c(x_{N-1}, x_{N-1})] - [c(x_0, x_{N-1}) - c(x_{N-1}, x_{N-1})] \\ &\quad + [c(x_{N+1}, x_N) - c(x_N, x_N)] \\ &\leq c(x_N, x_{N-1}) - c(x_0, x_{N-1}) + c(x_0, x_N) - c(x_N, x_N) \\ &= - \int_{x_0}^{x_N} \int_{x_{N-1}}^{x_N} \frac{\partial^2 c}{\partial x \partial y}(x, y) dy dx \leq 0, \end{aligned}$$

which completes the proof. \square

The sine example

Now we can turn our view on a particular result from Uckelmann [46], see Rüschendorf & Uckelmann [41] as well, which somehow perfectly matches the sine question. It is an open problem from [43]) which could not be treated by direct analytical methods.

For dealing with this example one may utilize a modification of Theorem 1. from [46]. We re-state the following version of this result and sketch its proof.

Remark 3.3

In this particular setting it is possible to construct explicitly an c -convex function f such that Theorem 3.5 can be used to deduce the optimal transport plan, i.e. optimal coupling. Notice, see [39], that $y \in \partial_c f(x)$ if and only if $\exists a(= a(y)) \in \mathbb{R}$ such that

$$\psi_{y,a}(x) = c(x, y) + a(y) = f(x) \quad \text{and} \quad \psi_{y,a}(\xi) = c(\xi, y) + a(y) \leq f(\xi) \quad \forall \xi \in X. \quad (10)$$

Theorem 3.7

Let μ, ν be the uniform distribution on $[0, 1]$ and the cost function $c(x, y) = \phi(x + y)$ with $\phi : [0, 2] \rightarrow \mathbb{R}$. In particular we assume that $\phi \in \mathcal{C}^2[0, 1]$ and that there is $k \in (0, 2)$ such that $\phi''(x) < 0$ for $x \in [0, k]$ and $\phi''(x) > 0$ for $x \in (k, 2]$. If $\beta \in (0, 1)$ denotes the solution to

$$\phi(2\beta) - \phi(\beta) = \beta\phi'(\beta),$$

then

$$\Gamma(x) = \begin{cases} \beta - x, & x \in [0, \beta), \\ x, & x \in [\beta, 1], \end{cases}$$

induces by $(U, \Gamma(U))$ for some standard uniformly distributed U an optimal c -coupling between P and Q .

Proof: For the proof we proceed as proposed in [46] and [41]. Define the following functions:

$$\begin{aligned} f_1(x) &= x\phi'(\beta), \\ f_2(x) &= \frac{1}{2}(\phi(2x) - \phi(2\beta)) + \beta\phi'(\beta), \\ \psi^1(\xi) &= \phi(\beta - x + \xi) + x\phi'(\beta) - \phi(\beta), \\ \psi^2(\xi) &= \phi(x + \xi) - \frac{1}{2}\phi(2x) - \frac{1}{2}\phi(2\beta) + \beta\phi'(\beta). \end{aligned}$$

Furthermore set

$$f(x) = f_1(x)I_{[0,\beta)}(x) + f_2(x)I_{[\beta,1]}(x),$$

and put for $\xi \in [0, 1]$:

$$\psi_{\Gamma(x)}(\xi) = \begin{cases} \psi^1(\xi), & x \in [0, \beta), \\ \psi^2(\xi), & x \in [\beta, 1]. \end{cases}$$

Here $\psi_{\Gamma(x)}(\xi)$ plays the role of $\psi_{y,a}(\xi) = c(\xi, y) + a(y)$ with $y = \Gamma(x)$ in (10). Now the idea, following Theorem 3.5 and (10), is to show that $y = \Gamma(x)$ is in the c -subdifferential of $f(x)$ for all $x \in [0, 1]$ which implies optimality of this particular coupling and optimality of the distribution induced by $(U, \Gamma(U))$ for the transport problem. For the c -convexity of f and the subdifferential property we need to show:

$$\begin{aligned} \psi_{\Gamma(x)}(x) &= f(x) \quad \forall x \in [0, 1], \\ \psi_{\Gamma(x)}(\xi) &\leq f(\xi) \quad \forall \xi \in [0, 1]. \end{aligned}$$

We start with showing that $\psi_{\Gamma(x)}(x) = f(x)$. For $x \in [0, \beta)$ we have that $\Gamma(x) = \beta - x$ and

$$\psi_{\Gamma(x)}(x) = \psi^1(x) = x\phi'(\beta) = f_1(x) = f(x).$$

For $x \in [\beta, 1]$ we have $\Gamma(x) = x$ and

$$\psi_{\Gamma(x)}(x) = \psi^2(x) = \frac{1}{2}(\phi(2x) - \phi(2\beta)) + \beta\phi'(\beta) = f_2(x) = f(x).$$

It remains to show $\psi_{\Gamma(x)}(\xi) \leq f(\xi)$ for all $(x, \xi) \in [0, 1] \times [0, 1]$, which can be achieved by a rather lengthy and carefull analysis, for the details see [4]. \square

Remark 3.4

If $\beta > 1$ then it can be shown as in the first step of the above proof that $(U, 1 - U)$ yields the optimal coupling. Loosely speaking one could say that the concave behaviour dominates the convex one.

Now we are prepared to answer the sine question. Setting $\phi(z) = \sin(\pi z)$ and $k = 1$ we immediately get:

Corollary 3.8

For $c(x, y) = \sin(\pi(x + y))$ we have that the distribution of the vector $(U, \Gamma(U))$ for $U \sim \mathcal{U}([0, 1])$ with

$$\Gamma(x) = \begin{cases} \beta - x, & x \in [0, \beta), \\ x, & x \in [\beta, 1], \end{cases}$$

and $\beta = 0.7541996008265638 \approx 0.7542$ which solves

$$\sin(2\pi\beta) - \sin(\pi\beta) = \beta\pi \cos(\pi\beta), \tag{11}$$

is maximizing

$$\int_{[0,1]^2} \sin(\pi(x+y)) d\gamma(x,y)$$

in the set of all bivariate distributions γ with uniform marginals, i.e., in the set of all copulas.

Remark 3.5

In this situation equation (11) meets the first order condition when looking at couplings of the form $(U, \Gamma^\alpha(U))$ with

$$\Gamma^\alpha(x) = \begin{cases} \alpha - x, & x \in [0, \alpha), \\ x, & x \in [\alpha, 1], \end{cases}$$

or explicitly maximizing $(c(x, y) = \sin(\pi(x + y)))$

$$H(\alpha) := \int_0^\alpha c(x, \alpha - x) dx + \int_\alpha^1 c(x, x) dx.$$

4 Approximations

In this section we are going to introduce some implementable approximation methods for the optimal transport problem. Since the computational methods are based on the *assignment problem*, see Burkard et al. [13], we recapitulate it and mention (some) one of the fundamental numerical solution algorithm(s). Some connections between the particular *copula maximization* problem and the assignment problem are already given in [25]. There the authors showed that for a piecewise constant cost function the maximizing measure is induced by a shuffle of M whose parameters are linked to the permutation which solves the corresponding assignment problem.

The (linear sum) assignment problem from combinatorial optimization is given by a matrix $(c_{ij})_{1 \leq i, j \leq n}$ with entries $c_{ij} \in \mathbb{R}$ which represent costs when assigning j to i , or when transporting 1 unit of mass from i to j . The goal is to match each row to a different column at minimal cost,

$$\sum_{i=1}^n \sum_{j=1}^n c_{ij} x_{ij} \rightarrow \text{minimum}$$

under the constraints $\sum_{j=1}^n x_{ij} = 1$ for $i \in \{1, \dots, n\}$, $\sum_{i=1}^n x_{ij} = 1$ for $j \in \{1, \dots, n\}$ and $x_{ij} \in \{0, 1\}$ for all $i, j \in \{1, \dots, n\}$. An interesting remark is given in [13, p. 75], it states that the problem above is equivalent to its continuous relaxation with $x_{ij} \geq 0$ for all $i, j \in \{1, \dots, n\}$.

Notice that if specifying $\mu = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$, $\nu = \frac{1}{n} \sum_{j=1}^n \delta_{y_j}$ for points $\{x_1, \dots, x_n\}$, $\{y_1, \dots, y_n\}$ in the unit interval and identifying $c(x_i, y_j) = c_{ij}$ one recovers exactly the assignment problem from the original transport problem. This connection also represents the first step in the proof of the fundamental Theorem 5.20 from [49].

Remark 4.1

As mentioned above a standard reference, from the theoretical as well as from the algorithmic point of view, is Burkard et al. [13]. Another reference for so-called quadratic assignment problems, incorporating a different cost structure, is Çela [16]. In the paper by Beiglöck et al. [9] the general duality theory of the transport problem is motivated by an explicit study of the assignment problem.

The assignment problem was among the first linear programming problems to be studied extensively. Given n workers and n jobs, we know, for every job, the salary that should be paid to each worker for him to perform the job. The goal is to find the the best assignment, i.e. each worker is assigned to exactly one job and vice versa in order to minimize the total cost (the sum of the salaries).

One of the many algorithms which solves the linear assignment problem is due to Kuhn [28] and Munkres [32] (also known as the Hungarian method).

In fact the algorithm was developed and published by Kuhn [28], who gave the name “Hungarian method”. Munkres [32] reviewed the algorithm and observed that it is strongly polynomial.

The problem is formulated as follows: given n workers and tasks, and an $n \times n$ matrix containing the cost of assigning each worker to a task, find the cost minimizing assignment.

First the problem is written in the following matrix form

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \ddots & & \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix},$$

where the $a_{i,j}$ ’s denote the penalties incurred when worker i performs task j .

The first step of the algorithm consists in subtracting the lowest $a_{i,j}$ ’s of the i th row from each element in that row. This will lead to at least one zero in that row. This procedure is repeated for all rows. We now have a matrix with at least one zero per row. We repeat this procedure for all columns (i.e. we subtract the minimum element in each column from all the elements in that column).

Then, we draw lines through the rows and columns so that all the zero entries of the matrix are covered and the minimum number of such lines is used. Finally, we check if an optimal assignment is possible. If the minimum number of covering lines is exactly n , an optimal assignment of zeros is possible and we are finished. Otherwise, if the minimum number of covering lines is less than n , an optimal assignment of zeros is not yet possible and we determine the smallest entry not covered by any line. We again subtract this entry from each uncovered row, and then add it to each covered column and we perform again the optimality test.

Due to its several applications and to the possible connections with related problems, many researchers got interested in the higher dimensional version of the linear assignment problem, the MAP, where one aims to find tuples of elements from given sets, such that the total cost of the tuples is minimal. While the linear assignment problem is solvable in polynomial time, the MAP is NP-hard (see e.g. [13]). Recently, a new approach based on the Cross-Entropy (CE) methods has been developed in [34] for solving the MAP. The efficiency of this method is corroborated by several teCsts on large-scale problems.

4.1 Theoretical basis

For computational purposes the following fairly general result due to Schachermayer & Teichmann [42] is valuable.

Theorem 4.1 (Th. 3 from [42])

Let $c : X \times Y \rightarrow \mathbb{R}_{\geq 0}$ be a finitely valued, continuous cost function on Polish spaces X, Y . Let $\{\pi_n\}_{n \geq 0}$ be an approximating sequence of optimizers associated to weakly converging sequences $\mu_n \rightarrow \mu$ and $\nu_n \rightarrow \nu$ as $n \rightarrow \infty$, i.e., π_n being an optimizer for the transport problem (c, μ_n, ν_n) . Then there is a subsequence $\{\pi_{n_k}\}_{k \geq 0}$ converging weakly to a transport plan π on $X \times Y$, which optimizes the Monge-Kantorovich problem for (μ, ν, c) . Any other converging subsequence of

$\{\pi_n\}_{n \geq 0}$ also converges to an optimizer of the Monge-Kantorovich problem, i.e., the non-empty set of adherence points of $\{\pi_n\}_{n \geq 0}$ is a set of optimizers.

An approximation result suited for the uniform marginals situation is Theorem 2.2 from [25], here we can complement it by proving that a (sub-)sequence of the discrete optimizers converges to an optimizer of the limiting continuous problem.

Theorem 4.2

Let c be a continuous function on $[0, 1]^2$, let the sets $I_{i,j}^n$ be given as

$$I_{i,j}^n = \left[\frac{i-1}{2^n}, \frac{i}{2^n} \right] \times \left[\frac{j-1}{2^n}, \frac{j}{2^n} \right] \text{ for } i, j = 1, \dots, 2^n,$$

for every $n > 1$ and define the functions $\underline{c}_n, \bar{c}_n$ as

$$\begin{aligned} \underline{c}_n(x, y) &= \min_{(x,y) \in I_{i,j}^n} c(x, y), \quad \text{for all } (x, y) \in I_{i,j}^n, \\ \bar{c}_n(x, y) &= \max_{(x,y) \in I_{i,j}^n} c(x, y), \quad \text{for all } (x, y) \in I_{i,j}^n. \end{aligned} \quad (12)$$

Furthermore, let $\underline{\gamma}_{\max}^n, \bar{\gamma}_{\max}^n$ be maximizing measures for cost functions \underline{c}_n and \bar{c}_n respectively. Then

$$\begin{aligned} \lim_{n \rightarrow \infty} \int_{[0,1]^2} \underline{c}_n(x, y) \underline{\gamma}_{\max}^n(dx, dy) &= \lim_{n \rightarrow \infty} \int_{[0,1]^2} \bar{c}_n(x, y) \bar{\gamma}_{\max}^n(dx, dy) \\ &= \sup_{\gamma \in \mathcal{C}} \int_{[0,1]^2} c(x, y) \gamma(dx, dy). \end{aligned} \quad (13)$$

Furthermore the sequence of maximizers converges, at least along some subsequence, to a maximizer of the original problem $\int_{[0,1]^2} c \gamma(dx, dy)$.

Proof: The first statement (13) is already shown in [25]. For the remaining part we can proceed in the spirit of Villani's proof of Theorem 5.20 from [49], notice there a sequence of continuous functions c_n is considered. We will show the proof for the lower approximation via \underline{c}_n .

At first observe that $\underline{\gamma}^n$ converges (at least along some subsequence) to some measure γ^* with uniform marginals, cf. [27, Thm. 5.21].

From above we know that $\underline{\gamma}^n$ is concentrated on a \underline{c}_n -cyclically monotone set with the consequence that for some $N \in \mathbb{N}$ the N -fold product measure $\underline{\gamma}^{n, \oplus N}$ is concentrated on the set $\mathcal{S}_n(N)$ of points $(x_1, y_1), \dots, (x_N, y_N)$ for which

$$\sum_{j=1}^N \underline{c}_n(x_j, y_j) \geq \sum_{j=1}^N \underline{c}_n(x_{j+1}, y_j),$$

with $x_{N+1} = x_1$. Now fix some $\varepsilon > 0$ and choose n large enough, such that $\underline{\gamma}^{n, \oplus N}$ is concentrated on the set $\mathcal{S}_\varepsilon(N)$ of points with

$$\sum_{j=1}^N c(x_j, y_j) \geq \sum_{j=1}^N c(x_{j+1}, y_j) - \varepsilon.$$

Since c is continuous we have that $\mathcal{S}_\varepsilon(N)$ is a closed set. This (using indicator functions in the weak convergence characterization) implies that also the limiting measure $\gamma^{*, \oplus N}$ is concentrated on $\mathcal{S}_\varepsilon(N)$ for all $\varepsilon > 0$. We can let $\varepsilon \rightarrow 0$ and derive that $\gamma^{*, \oplus N}$ is concentrated on a set of points with

$$\sum_{j=1}^N c(x_j, y_j) \geq \sum_{j=1}^N c(x_{j+1}, y_j)$$

and therefore is concentrated on a c -cyclically monotone set. Since the costs are bounded we deduce from Theorem 3.4(b) that γ^* is optimal. \square

Remark 4.2

Theorem 4.1 can be used when approximating μ and ν by empirical distributions. Let X_1, X_2, \dots be i.i.d. random variables with distribution μ and Y_1, Y_2, \dots be i.i.d. random variables with distribution ν . Then the empirical distributions defined by $\hat{\mu}_n(-\infty, x] = \frac{1}{n} \sum_{k=1}^n I_{\{X_k \leq x\}}$ and $\hat{\nu}_n(-\infty, x] = \frac{1}{n} \sum_{k=1}^n I_{\{Y_k \leq x\}}$ converge weakly to μ and ν , see [27, Prop. 4.24]. In this situation one can solve assignment problems along realizations of the random sequences $\{X_k\}$ and $\{Y_k\}$.

The spirit of Theorem 4.2 is a little different. There the marginal distributions are fixed to be uniform, whereas the cost function is approximated by piecewise constant functions on a deterministically chosen grid. This particular situation is linked to a solution of the assignment problem via Theorem 2.1 of [25].

4.2 Numerical examples

An explicit implementation of the Hungarian algorithm applied to the cost function $c(x, y) = \sin(\pi(x + y))$ can be found in [25]. The authors provide also a numerical solution to a problem in financial mathematics, namely the First-to-Default (FTD) swap. This is a contract between an insurance buyer and an insurance seller. The first one makes periodic premium payments, called spreads, until the maturity of the contract or the default, whichever occurs first. In exchange the second one compensates the loss caused by the default at the time of default. In [25] an approximation of the value of the maximal spread is provided.

Of course other applications are possible and interesting, but this goes beyond the purposes of the present paper.

Our aim is to consider some cost functions c involving the sine function as in [25] and to show how the support of the copula where the maximum is attained can vary considerably. More precisely, we consider

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N c(x_n + y_n), \quad (14)$$

with $c(x, y) = \sin(2\pi x) \sin(2\pi y)$, $c(x, y) = \sin(2\pi x) \cos(2\pi y)$ and $c(x, y) = \sin(2\pi/x) \cos(2\pi y)$. In particular, the numerical costs for the transport map in the first case is 0.5, which is the same as when using the identity map (explicitly computed). Let us remark that obviously there is no unique solution.

The numerical results are illustrated in Table 1.

$n \backslash c$	$\sin(\pi x) \sin(\pi y)$	$\sin(\pi x) \cos(\pi y)$	$\sin(\pi/x) \cos(\pi y)$
2	0.5	0.1768	0.4612
3	0.5	0.2039	0.3402
4	0.5	0.2102	0.5067
5	0.5	0.2117	0.4012
6	0.5	0.2121	0.4580
7	0.5	0.2122	0.4400

Table 1: Upper bounds for the lim sup in (14).

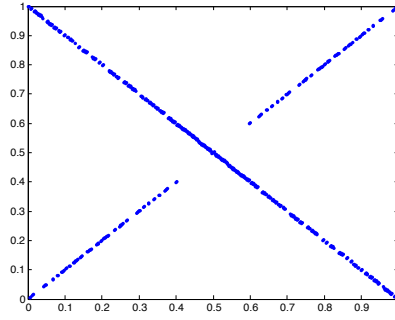


Figure 1: Support of copula which attains upper bound for $c(x, y) = \sin(\pi x) \sin(\pi y)$ and $n = 10$

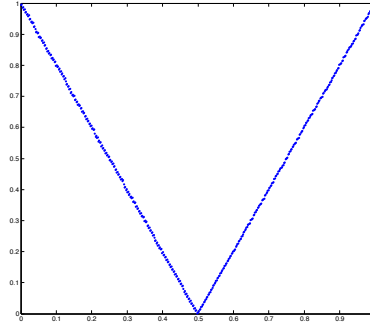


Figure 2: Support of copula which attains upper bound for $c(x, y) = \sin(\pi x) \cos(\pi y)$ and $n = 10$

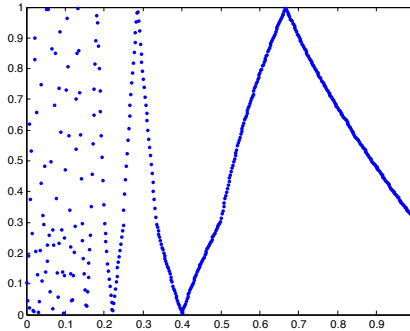


Figure 3: Support of copula which attains upper bound for $c(x, y) = \sin(\pi/x) \cos(\pi y)$ and $n = 10$

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